Sheryl P. Walter Declassified/Released US Department of State EO Systematic Review 20 Mar 2014

Message Text

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TAGS: TPHY, OSCI, TBIO, IN

SUBJECT: DHEW/PHS/NIH - TRANSMITTAL OF EVALUATION OF
THESIS SUBMITTED BY CHANCHAL K. MITRA

PASS TO SCIATT. ATTENTION MR. M. L. SAXENA

1. EMBASSY IS REQUESTED TO TRANSMIT PROMPTLY THE FOLLOW-
ING MESSAGE TO PROFESSOR GIRJESH GOVIL, TATA INSTITUTE OF
FUNDAMENTAL RESEARCH, BOMBAY. IT IS AN EVALUATION OF A
DOCTORAL THESIS OF A CANDIDATE SCHEDULED FOR AN IMMINENT
EXAMINATION AND DEFENSE OF HIS THESIS. DR. GOVIL SHOULD
BE INFORMED THAT THIS EVALUATION WAS MADE BY DR. TODD MILES.

2. QUOTE REPORT ON THESIS SUBMITTED BY C. K. MITRA. IN
MY OPINION THE THESIS 'THEORETICAL STUDIES ON STRUCTURE
AND FUNCTION OF BIOMOLECULES' BY CHANCHAL MITRA MAKES AN
INVALUABLE CONTRIBUTION TO OUR UNDERSTANDING OF SEVERAL
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CLASSES OF BIOLOGICALLY IMPORTANT MOLECULES. THESE
INCLUDE THE NATURALLY OCCURING NUCLEOSIDES, SELECTED
NUCLEOSIDE ANALOGS, 6-AZAPYRIMIDINE NUCLEOSIDES,
8-AZAPURINE NUCLEOSIDES, AND SEVERAL NUCLEOSIDE
ANTIBIOTICS.

3. THE THEORETICAL BACKGROUND IS SYSTEMATICALLY DEVELOPED

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AND CLEARLY PRESENTED. AS AN EXPERIMENTAL CHEMIST WORKING IN THE FIELD OF NUCLEOTIDES AND POLYNUCLEOTIDES, I AM IMPRESSED AT HOW WELL THE AUTHOR CONVEYS THE IDEAS TO SOMEONE RELATIVELY UNFAMILIAR WITH THE THEORETICAL METHODS EMPLOYED. A STRONG POINT OF THE THESIS IS THE CONSISTENT EVALUATION OF THEORETICAL RESULTS AGAINST THE AVAILABLE EXPERIMENTAL EVIDENCE, IN MY VIEW AN ESSENTIAL PART OF THEORETICAL STUDIES OF MOLECULES AS COMPLEX AS THOSE INVESTIGATED HERE. STRUCTURES OF THE MOLECULES SELECTED FOR STUDY HAD BEEN DETERMINED CRYSTALLOGRAPHI-CALLY, PROVIDING COORDINATES FOR INITIAL INPUT AND EXPERIMENTAL DATA FOR COMPARISON WITH THE CALCULATED RESULTS. WHEN THE STRUCTURE CORRESPONDING TO THE GLOBAL ENERGY MINIMUM DIFFERS FROM THE CRYSTALLOGRAPHIC STRUCTURE, AS IT OFTEN DOES, EXPLANATIONS ARE SOUGHT IN TERMS OF ENVIRONMENTAL FACTORS SUCH AS CRYSTAL PACKING, INTERMOLECULAR, AND INTRAMOLECULAR HYDROGEN BONDING. VARIATION OF STRUCTURE UNDER THE INFLUENCE OF SUCH INTERACTIONS IS A MATTER OF MAJOR CONCERN TO CHEMISTS, AND THE CALCULATIONS DESCRIBED IN THIS THESIS PROVIDE RELEVANT INSIGHT, OFTEN IN AREAS WHICH ARE EXPERIMENTALLY INACCESSIBLE. IT IS UPON THE FLEXIBILITY OF THESE MOLECULES, ACHIEVED THROUGH SINGLE BOND TORSIONS, THAT MANY OF THEIR MOST IMPORTANT CHEMICAL AND BIOLOGICAL PROPERTIES DEPEND. I BELIEVE THIS STUDY IS OF MAJOR
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VALUE IN ELUCIDATING THE FACTORS GOVERNING THE FLEXIBILITY AND SHAPE OF THESE IMPORTANT BIOMOLECULES. UNQUOTE. CHRISTOPHER

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